

Jurs-RASA—16.827%; Jurs-PPSA-1—15.494%; Jurs-TPSA—10.218%; Jurs-RPSA—5.444%; Hbond donor—3.905%; Hbond acceptor—3.729%; Jurs-FPSA-1—3.409%; Fcharge—2.892%; Jurs-PNSA-1—1.244%; RadOfGyration—1.164%; Rotbonds—1.156%; Apol—1.148%; Jurs-PPSA-2—1.016%; Jurs-PNSA-2—0.632%; Jurs-RNCG—0.400%; Dipole-mag—0.298%; Jurs-FNSA-3—0.127%; A log P—0.051%; Conformer Energy—0.037%; Jurs-RPCG—0.024%; and Jurs-DPSA-2—0.00%.

**23.** A method for determining whether a synthetic peptide is bioactive against *Staphylococcus aureus* (SA), comprising the steps of:

- i) determining the shape of a peptide that has minimum potential energy of the peptide;
- ii) computing the conformational model for the peptide using standard Monte Carlo or molecular dynamics conformational search algorithms, so as to generate a pool of peptide conformations that are within 20 Kcals/mol energy range of the global minimum conformation;
- iii) selecting from the peptide conformations of step ii) the conformation having the maximum measurement of its backbone when measured from head to tail, which conformation is within five Kcals/mole energy range of the global minimum conformer;
- iv) aligning all conformations of step ii) with the selected conformation of step iii), wherein the selected conformation is used as a template structure;
- v) determining the physicochemical properties for all the aligned conformations, wherein the physicochemical properties determined are conformer energy, Fcharge, dipole-mag, Jurs-SASA, Jurs-PPSA-1, Jurs-PNSA-1, Jurs-PNSA-2, Jurs-DPSA-2, Jurs-DPSA-3, Jurs-FPSA-1, Jurs-FPSA-3, Jurs-FNSA-3, Jurs-RPCG, Jurs-RPCS, Jurs-TASA, Jurs-RPSA, Jurs-RASA, density, Hbond acceptor, Hbond donor, Rotbonds, A log P, and RadOfGyration; and
- vi) applying a mathematical equation to each aligned conformation peptide, to *Staphylococcus aureus* (SA), which mathematical equation is: SA bioactivity equals satisfaction of at least four of the following terms:  $[( -1.49592 \times "Fcharge") + (0.0098147 \times "dipole-mag") + (0.013993 \times "Jurs-SASA") + (0.00233 \times "Jurs-PPSA-1") + (0.187647 \times "Jurs-PNSA-1") + (0.0021686 \times "Jurs-PNSA-2") + (0.00036919 \times "Jurs-DPSA-2") + (0.0015025 \times "Jurs-DPSA-3") + (438.251 \times "Jurs-FPSA-1") + (267.258 \times "Jurs-FPSA-3") + (120.432 \times "Jurs-FNSA-3") - (715.316 \times "Jurs-RPCG") - 12.8649 \times "Jurs-RPCS") - (0.065752 \times "Jurs-TASA") - (125.513 \times "Jurs-RPSA") + (125.513 \times "Jurs-RASA") - (183.99 \times "density") + (1.03397 \times "Hbond acceptor") + (0.039473 \times "Hbond donor") - (0.306856 \times "Rotbonds") + (0.114808 \times "A log P") - (0.10004 \times "RadOfGyration") - 225.589]$ .

**24.** A method for determining whether a synthetic peptide is bioactive against *Mycobacterium ranae* (MR), comprising the steps of:

- i) determining the shape of a peptide that has minimum potential energy of the peptide;
- ii) computing the conformational model for the peptide using standard Monte Carlo or molecular dynamics conformational search algorithms, so as to generate a pool of peptide conformations that are within 20 Kcals/mol energy range of the global minimum conformation;
- iii) selecting from the peptide conformations of step ii) the conformation having the maximum measurement of its backbone when measured from head to tail, which conformation is within five Kcals/mole energy range of the global minimum conformer;
- iv) aligning all conformations of step ii) with the selected conformation of step iii), wherein the selected conformation is used as a template structure;
- v) determining the physicochemical properties for all the aligned conformations, wherein the physicochemical properties determined are conformer energy, Fcharge, Apol, dipole-mag, Jurs-PPSA-1, Jurs-PNSA-1, Jurs-PPSA-2, Jurs-PNSA-2, Jurs-FPSA-1, Jurs-FNSA-3, Jurs-RPCG, Jurs-RNCG, Jurs-TPSA, Jurs-RPSA, Jurs-RASA, density, Hbond acceptor, Hbond donor, Rotbonds, A log P, and RadOfGyration; and
- vi) applying a mathematical equation to each aligned conformation peptide, to determine whether the synthetic peptide is bioactive against *Mycobacterium ranae* (MR), which mathematical equation is: MR bioactivity equals satisfaction of at least four of the following terms:  $[( -0.0083585 \times "conformer energy") + (2.05758 \times "Fcharge") + (5.3259e-05 \times "Apol") + (0.0061422 \times "dipole-mag") - (0.023941 \times "Jurs-PPSA-1") - (0.008252 \times "Jurs-PNSA-1") + (5.5381e-05 \times "Jurs-PPSA-2") + (0.00018566 \times "Jurs-PNSA-2") - (18.282 \times "Jurs-FPSA-1") + (13.321 \times "Jurs-FNSA-3") - (8.46841 \times "Jurs-RPCG") + (66.6262 \times "Jurs-RNCG") + (0.052889 \times "Jurs-TPSA") - (96.9761 \times "Jurs-RPSA") + (96.9761 \times "Jurs-RASA") - (127.577 \times "density") + (0.768698 \times "Hbond acceptor") - (0.498282 \times "Hbond donor") - (0.060764 \times "Rotbonds") - (0.075759 \times "A log P") + (0.337835 \times "RadOfGyration") + 110.841]$ .

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